

Numerical studies of various Néel-VBS transitions in $SU(N)$ anti-ferromagnets

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Abstract. In this manuscript we review recent developments in the numerical simulations of bipartite $SU(N)$ spin models by quantum Monte Carlo (QMC) methods. We provide an account of a large family of newly discovered sign-problem free spin models which can be simulated in their ground states on large lattices, containing $O(10^5)$ spins, using the stochastic series expansion method with efficient loop algorithms. One of the most important applications so far of these Hamiltonians are to unbiased studies of quantum criticality between Néel and valence bond phases in two dimensions – a summary of this body of work is provided. The article concludes with an overview of the current status of and outlook for future studies of the “designer” Hamiltonians.

1. Overview

The study of ground states of lattice models of quantum spins has become a major field in condensed matter physics [1]. Despite their simplicity these models can be extremely hard to study theoretically, due in part to the rich variety of ground states that they can host. Recent years have seen a dramatic increase in the use of numerical methods to study the ground states of quantum spin models. Of particular interest are “unbiased” numerical methods, which solve for physical properties of model systems with numerical errors that can be controlled and estimated in a reliable fashion. Quantum Monte Carlo occupies a special place among the unbiased methods because when applicable, it is the only technique that is able to access the large systems sizes required for reliable extrapolation to the thermodynamic limit, especially in the proximity of critical phenomena [2].

The simplest ground state that can arise in a quantum spin system is a magnetic ground state, where the expectation value of the spin on a site is finite, causing the spin to effectively “point” in a certain direction, thus spontaneously breaking the global symmetry associated with the rotation of spins. Such magnetic states are well known to arise in the low-energy space of classical spin models and their appearance in quantum models can be understood from semi-classical arguments. The focus of recent numerical studies of spin models has been in large part on the nature of the *non-magnetic phases* that arise at $T = 0$ due to quantum fluctuations and the quantum phase transitions separating magnetic and non-magnetic phases. The non-magnetic

phases may either break another symmetry, most often a lattice translational symmetry in which case they are called “solids” or be completely symmetric in both the lattice and spin symmetries in which case they are called “liquids.” The central questions of interest to numerical studies are: What is the precise characterization of the non-magnetic phases, both of the “solid” and “liquid” type that are found in simple microscopic models? How can the phase transitions between the magnetic and non-magnetic phases observed in numerical simulations be understood in terms of long wavelength quantum field theories?

While these general questions have received copious attention from a multitude of complementary approaches in different contexts over the last three decades [2, 3, 4, 5], in this review we will outline how new “designer” Hamiltonians with $SU(N)$ symmetry have contributed to answers concerning phase transitions between $SU(N)$ symmetry breaking magnetic phases and lattice translational symmetry breaking valence-bond solid states, for which an exotic direct continuous transition – “deconfined criticality” – has been proposed [6, 7, 8]. For a fuller appreciation of this short review, a familiarity with the deconfined theory is recommended. In the interest of space this is not provided here, the interested reader is encouraged to refer to the original literature. In Section 2 we briefly review the discovery of a large family of “designer” $SU(N)$ models that do not suffer from the sign problem. In Sec 3 we describe the phase diagrams obtained for the Hamiltonians that have been studied so far and the nature of the critical points that arise between different phases. Finally, in Section 4 we conclude with an outlook and directions for future work.

2. $SU(N)$ Hamiltonians, loop models and the sign problem

In order to use unbiased quantum Monte-Carlo techniques efficiently, one needs to identify models that do not suffer from the sign problem. It is well known that Hamiltonians that satisfy Marshall’s sign condition are also sign-problem free. So a basic questions of central importance to the numerical simulations of quantum spin models is: What is the family of spin models that satisfies Marshall’s sign criteria?

In order to make this question concrete, we specialize our considerations to bipartite models with a specific representation of $SU(N)$ symmetry, originally introduced to condensed matter physics by Affleck [9]. This realization of $SU(N)$ symmetry requires spins on one sub-lattice to transform in the fundamental representation of $SU(N)$ and spins on the other sub-lattice to transform in the conjugate to fundamental representation. We note here for $N = 2$, since the fundamental and conjugate to fundamental representations are identical, this realization of $SU(2)$ symmetry gives rise to the familiar Heisenberg-like models.

The standard quantum-classical mapping allows us to rewrite the quantum statistical mechanics of d -dimensional Hamiltonians as a classical statistical mechanics problem in $d + 1$ -dimensions, where the extra dimension is of extent $\beta = 1/T$. The stochastic series expansion (SSE) is an elegant and well-documented method to execute this step [10]. When carried out and as discussed in detail [11], the Affleck $SU(N)$ spin models on bipartite lattices can be mapped to *oriented tightly packed loop models with N colors* in one higher dimension. In order to carry out Monte Carlo sampling we require these configurations to have positive weights. In the language of loop models it is straightforward to systematically write down all possible interactions that keep the weights of the loop configurations positive. When the quantum-classical mapping is run backwards, the interactions in the classical loop model correspond to terms in quantum Hamiltonians that are Marshall positive. This picture allows one to systematically write down a large class of $SU(N)$ spin Hamiltonians that are Marshall positive. We note parenthetically that the Marshall positivity of these “designer” Hamiltonians is not obvious when viewed directly in the spin language, and that the “designer” models include all previously known Marshall positive spin models as particular cases.

As a concrete example of the results, let us discuss the familiar $N = 2$ case. Here the spins

\vec{S} on either sub-lattice can be written in terms of Pauli matrices in the usual way. Previously known sign-problem-free Hamiltonians include (with $J_1, J_2, Q > 0$) [12],

$$\begin{aligned} H_{J_1} &= J_1 \vec{S}_1^A \cdot \vec{S}_1^B \\ H_{J_2} &= -J_2 \vec{S}_1^A \cdot \vec{S}_2^A \\ H_Q &= -Q \left(\vec{S}_1^A \cdot \vec{S}_1^B - \frac{1}{4} \right) \left(\vec{S}_2^A \cdot \vec{S}_2^B - \frac{1}{4} \right) \end{aligned} \quad (1)$$

where the superscript A, B indicates the sublattice the spin lives on and the subscript indicates the different spins on a given sublattice. Thus the J_1 interaction is defined on two spins, one of which lives on the A sublattice and the other on the B sublattice, the J_2 interaction is defined on two spins on the same sublattice, and the Q interaction is defined on four spins, two on the A sublattice and two on the B sublattice. As an application of the new strategy sketched above, a new linearly independent four-spin interaction can be shown to be Marshall positive,

$$\begin{aligned} H_R &= R \left(\vec{S}_1^A \cdot \vec{S}_2^A - \frac{1}{4} \right) \left(\vec{S}_1^B \cdot \vec{S}_2^B - \frac{1}{4} \right) \\ &- R \left(\vec{S}_1^A \cdot \vec{S}_1^B - \frac{1}{4} \right) \left(\vec{S}_2^A \cdot \vec{S}_2^B - \frac{1}{4} \right) - R \left(\vec{S}_1^A \cdot \vec{S}_2^B - \frac{1}{4} \right) \left(\vec{S}_1^B \cdot \vec{S}_2^A - \frac{1}{4} \right) \end{aligned} \quad (2)$$

It is straightforward to prove the Marshall positivity of the above interaction by direct evaluation of its matrix elements when $R > 0$, even though its positivity is not apparent from a naive inspection of the term.

We note following the strategy described in Ref. [11], all the Marshall-positive interactions involving an arbitrary large number of A and B spins and with any N (of $SU(N)$) can be systematically written down. Also from the way the interactions are written above it is clear that they can be written on any bipartite lattice in any dimension, and can be made to preserve the lattice symmetry through an appropriate summation over the entire lattice.

Detailed reviews and pedagogical introductions to the kind of QMC algorithms that are used to simulate the spin models introduced in this Section may be found in [10, 2].

3. Phase Diagrams & Quantum Criticality

The only two phases found so far in the numerical simulations of the bipartite $SU(N)$ sign-free models discussed in Sec. 2 are Néel and “valence-bond” phases (VBS). By “valence-bond” phases we mean phases that are smoothly connected to a product state of two-site valence bond coverings (see Fig. 1 for cartoons of such coverings). The numerical study of the Néel and VBS phases of the Affleck $SU(N)$ models was initiated early on [13, 14]. However, the most intriguing aspect of the phase diagram, the critical point, was first accessed with the introduction of the four-site Q interaction 1 for the $N = 2$ case [12]. While the pioneering study was carried out for $N = 2$ on the square lattice, subsequent work has carried out the study for a large range of N and for a variety of bipartite lattices and interactions.

In order to summarize the studies in “conceptual” rather than historical order, we need one technical result from the deconfined theory. The deconfined theory predicts that for bipartite $SU(N)$ magnets in two dimensions, the Néel-VBS critical point is described by a nc- \mathbb{CP}^{N-1} critical field theory, only for certain “columnar” VBS states. In actual lattice realization, whether in numerical simulations or real materials, a perturbation to the nc- \mathbb{CP}^{N-1} theory, λ_q (for the experts, it is the fugacity of q -monopoles in the gauge field) is present. The central difference between the various bipartite lattices is the integer q , which can be intuitively understood as the minimum degree of degeneracy of the VBS phase on the particular bipartite lattice under consideration. In order for the deconfined critical point to exist λ_q must be *irrelevant* at the

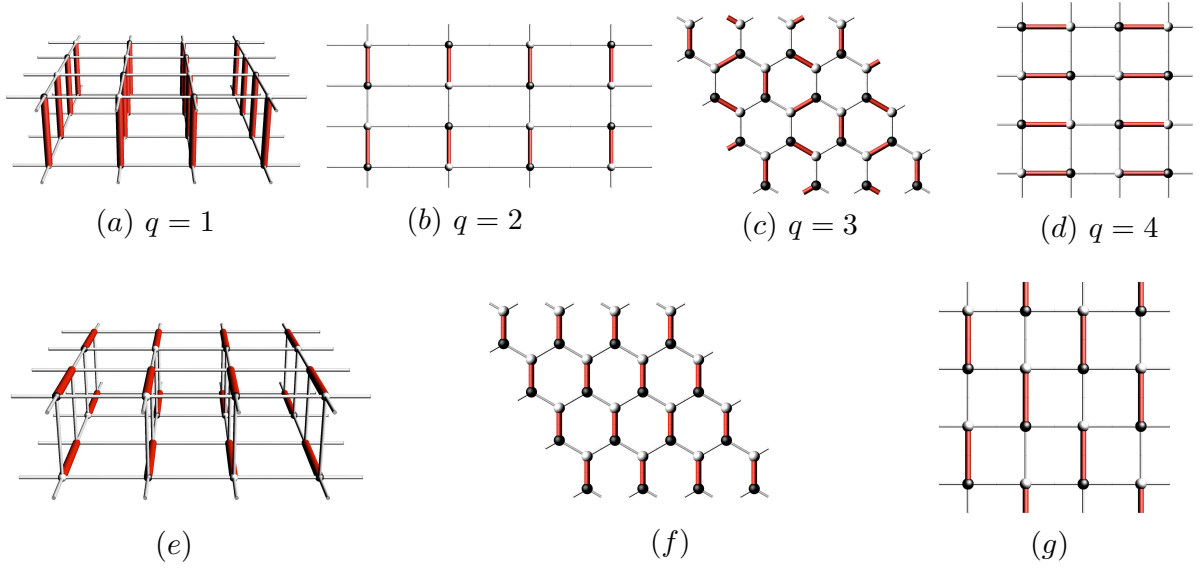


Figure 1. Summary of valence-bond patterns that have been accessed in numerical simulations of two-dimensional bipartite $SU(N)$ designer Hamiltonians. The quantum phase transition into each of these phases from $SU(N)$ symmetry breaking Néel phases is the subject of this review. The thick red bonds when put in an $SU(N)$ singlet state provide a cartoon state for the symmetry breaking. (a-d) are the “columnar” patterns for which the theory of a continuous deconfined criticality can hold for sufficiently large N . The value of q is the degeneracy of the VBS coverings in these states. (e) is a four-fold degenerate VBS state on a bilayer to which there is a first order transition. (f,g) are three- and four-fold staggered VBS states into which there are also first order transitions.

monopole-free fixed point. If it is relevant one expects a first order transition or a continuous transition in a universality class different from the $nc\text{-}\mathbb{CP}^{N-1}$ universality.

Let us begin with the case of the bilayer lattice. The simplest non-magnetic state in the bilayer system is a non-degenerate ($q = 1$) rung singlet state (see Fig. 1(a)). For $N = 2$ there is beautiful evidence that supports the theoretical expectation [15] that there is a continuous critical point between Néel and rung-singlet state in the $2 + 1$ -dimensional $O(3)$ universality class [16]. For $N \geq 4$ numerical simulations have found evidence for a first order transition, which is expected from Landau theory [17]. The case $N = 3$ appears to have either a very weakly first order or a continuous transition. The field theoretical scenario explaining a possible continuous $N = 3$ transition has been nicely summarized in Ref. [18]. Other numerical work has studied the Néel-VBS transition on the rectangular ($q = 2$) [19], honeycomb ($q = 3$) [19, 20, 21] and square ($q = 4$) [12, 22, 23, 24] lattices for a range of N by using a judicious choice of the designer couplings defined in Section 2. See Fig. 1(b-d) for cartoons of the VBS states. Both first order transitions for small N and continuous transitions for large N have been identified. The critical value of N at which the transition turns continuous decreases as q increases, as expected theoretically. The appearance of continuous and first-order transitions occur in a systematic way that can be attributed to whether the lattice anisotropy in the form of λ_q is relevant or irrelevant at the $nc\text{-}\mathbb{CP}^{N-1}$ fixed point. The results may be summarized in Table 1, which shows whether the deconfined critical point between an $SU(N)$ magnet and q -degenerate VBS state (when it is the minimum degeneracy on a particular lattice) is stable. We note that in the bilayer model

| | | | | | | | |
|-------------------|---------|---------|---------|---------|---------|--------------|----------------------|
| $N = \infty, 1/N$ | I | I | I | I | \dots | I | nc-CP^{N-1} |
| \dots | | | | | | | |
| $N = 10$ | R | I | I | I | | I | nc-CP^9 |
| $N = 9$ | R | I | I | I | | I | nc-CP^8 |
| $N = 8$ | R | I | I | I | | I | nc-CP^7 |
| $N = 7$ | R | I | I | I | | I | nc-CP^6 |
| $N = 6$ | R | I | I | I | | I | nc-CP^5 |
| $N = 5$ | R | I | I | I | | I | nc-CP^4 |
| $N = 4$ | R | I | I | I | | I | nc-CP^3 |
| $N = 3$ | R | R | I | I | | I | nc-CP^2 |
| $N = 2$ | R | R | I | I | | I | nc-CP^1 |
| $N = 1$ | R | R | R | I | | I | XY |
| $N = 0$ | R | R | R | R | | R | photon |
| | $q = 1$ | $q = 2$ | $q = 3$ | $q = 4$ | \dots | $q = \infty$ | |

Table 1. Table showing the inferred relevance (R) or irrelevance (I) of q -monopoles at the nc-CP^{N-1} fixed point, which various studies summarized in the text have allowed us to complete. Numerical simulations of the Néel-VBS transition in the models discussed here only allow studies for $N \geq 2$. The entries with R correspond to an unstable fixed point, and I to a stable fixed point allowing for deconfined criticality. At some currently unknown critical value of $N > 10$, the $q = 1$ case switches from R to I . Adapted from Ref. [19]

($q = 1$) the R is expected to turn to I at a finite value of N – analytic estimates from large- N theories suggest this happens around $N \approx 25$ [25]. However, such large values of N have not been accessed numerically yet. For the values of N for which there is a continuous transition, the critical exponents should not depend on the bipartite lattice geometry, since λ_q is irrelevant if there is a continuous transition. Numerical measurements for the anomalous dimension of the Néel and VBS fields are consistent with this expectation and are consistent with results from the analytic $1/N$ expansion as shown in Fig. 2

Having discussed the cases of a “columnar” VBS state to which the theory of deconfined criticality applies, it is also of interest to numerically study the Néel-VBS transition in situations where the deconfined criticality does *not* apply, as a non-trivial check on the theory. As we shall see in the examples below there are a number of different reasons why this can happen:

(1) In the bilayer geometry, consider the phase transition between a four-fold degenerate columnar VBS (c-VBS), see Fig. 1(e), and the $\text{SU}(N)$ Néel state. The c-VBS on the bilayer breaks exactly the same symmetries as the single-layer c-VBS state (see Fig. 1(d)) and thus one might conclude naively based on “Landau” theory that they are described by the same critical phenomena. However, it is well known that in the bilayer geometry the Berry phases that are crucial for deconfined criticality cancel between the layers, eliminating the possibility of an exotic continuous transition. Consistent with this expectation, numerical studies have found that the c-VBS-Néel transition in the bilayer is first order [17].

(2) Back to the single-layer case, one can tune designer coupling to favor spontaneous symmetry breaking different from the “columnar” states for which the original proposal of deconfined criticality was made [6]. Indeed, studies have been carried out for the transition between Néel and “staggered” VBS for $\text{SU}(2)$, on the square lattice by tuning a “designer” six-spin interaction [26] and on the honeycomb by tuning a four-spin interaction [27]. The theory of a continuous deconfined critical point does not generalize to the staggered VBS case, and in

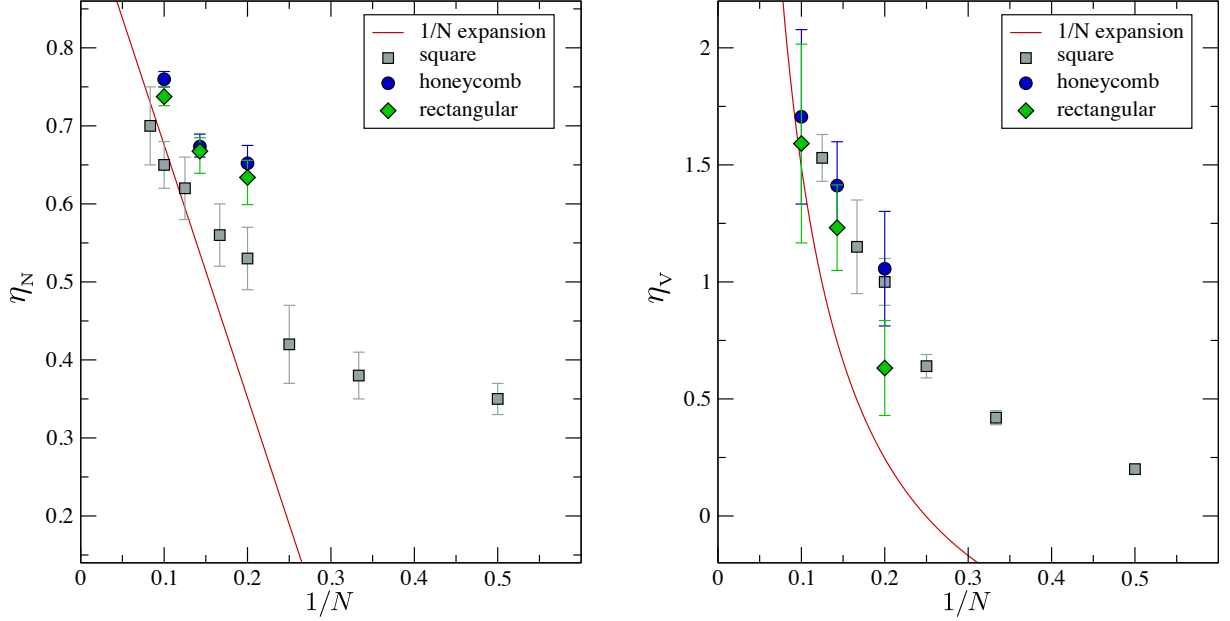


Figure 2. Comparison of anomalous dimensions of Néel and VBS operators in the case of continuous transitions for $q = 2, 3$ and 4 . (a) Anomalous dimension of the Néel order parameter as a function of $1/N$. (b) Anomalous dimension of the VBS order parameter as a function of $1/N$. The gray squares are the results of a square lattice study ($q = 4$) [22, 23]. The blue circles are results from the honeycomb lattice ($q = 3$) and the green diamonds are results from the rectangular lattice ($q = 2$). The red line is the $1/N$ expansion. The universality of the exponents with respect to q is a direct consequence of the irrelevance of λ_q . The agreement of the exponents with the $1/N$ computation is strong evidence for the emergence of the nc-CP^{N-1} universality at the Néel-VBS transition. Adapted from Ref. [19].

the absence of any plausible alternative one expects a restoration of “Landau” theory and hence a first-order transition. Consistently, both studies find clear evidence for first-order transitions between the Néel and staggered VBS phases.

(3) There have been two studies of the Néel-VBS transition in designer Hamiltonians in *three-dimensional* bipartite $\text{SU}(N)$ systems thus far. Both studies, which are on cubic lattices but with distinct Hamiltonians, find first-order transitions between Néel and columnar VBS and no evidence for any new intervening phases [28, 29]. The absence of a direct continuous transition in $3 + 1$ dimensions is again consistent with the deconfined criticality scenario since various aspects of the CP^{N-1} field theory are specific to $2 + 1$ dimensions and are known to be invalid in $3 + 1$ dimensions.

4. Outlook

In the previous section, we have summarized how the deconfined criticality scenario and the CP^{N-1} universality, convincingly explain unbiased numerical studies of the $\text{SU}(N)$ designer Hamiltonians in a variety of studies carried out by different groups, which have probed various distinct aspects of the deconfined criticality scenario.

One concern is that the transition could be weakly first order and the numerical studies, which are necessarily limited to finite size systems, may not have accessed sizes large enough to detect a first-order transition [30]. If this is indeed the case, the transition must be so weakly

first order that the correlation length exceeds the sizes of the largest lattices on which many of the designer Hamiltonians have been simulated, since no direct evidence for first-order behavior has been found in the cases where a continuous transition has been claimed. This makes the discussion of the presence of such a weakly first-order transition somewhat academic.

Nevertheless, there are well established corrections to scaling observed in the numerical studies of the Néel-VBS transition in the designer Hamiltonians [31, 32, 24, 21]. The origin of these corrections to the asymptotic behavior is not completely understood. Three options might be considered: (a) the transition is described completely by deconfined criticality; the corrections to scaling are just the usual corrections to asymptotic behavior that arise from deviants from the true fixed point due to irrelevant operators, finite size, etc. and will vanish in the thermodynamic limit; (b) the transition is weakly first order and no non-compact \mathbb{CP}^{N-1} fixed point exists; the deviation from scaling is claimed as incipient first order behavior; (c) there is something fundamentally new in the scaling behavior of deconfined critical points that needs to be understood; the “corrections” are part of the true asymptotic behavior and their existence can be understood from a field theoretic argument that has so far been overlooked.

Currently, it is not possible to rule out any of the three options categorically. Given the large body of evidence presented in Section 3 that appears consistent with the deconfined scenario and the lack of direct evidence for a first-order transition, Occum’s razor suggests that (a) is the most likely explanation. The corrections to scaling arising due to a irrelevant operator with a small exponent [33]. As a theoretical possibility, option (c) is the most exciting and is an interesting area for further field theoretic work [34, 35]. Likewise, some positive theoretical reasoning that supports the existence of a first-order transition and explains why it is so weak, or direct evidence numerical evidence for a first-order transition, would strengthen the case for option (b).

It is also possible that the transition is first order for small- N and becomes continuous only for some finite value of $N > 2$. Numerical studies on the designer Hamiltonians do not see a dramatic difference in the simulations between $N = 2$ and $N > 2$ for the cases where a continuous transition is found. It would be of interest to extend the studies of the $N = 2$ nc- \mathbb{CP}^{N-1} field theory on a lattice, to $N > 2$, which have not been carried out [30, 36].

Beyond the study of deconfined criticality, an as yet unanswered question is what other phases can be accessed in the family of sign-free $SU(N)$ spin models presented in Sec. 2. The only two phases found so far in these models are Néel and VBS phases, with the VBS phases being the simplest possible, i.e., they are each connected without phase transition to a cartoon state that is simply a direct product of two-site $SU(N)$ singlets. There is no evidence for plaquette VBS states in the designer models, despite many approximate studies favoring such a state in similar models. A related unanswered question is whether the $SU(N)$ “designer” Hamiltonians can host a spin liquid, and if so how to design such models. We note that Marshall positive models with simpler $U(1)$ symmetries have been shown convincingly to host Z_2 spin liquids [37, 38], but no such model with $SU(N)$ symmetry is known yet.

Finally, studies of the designer models with internal symmetries different from $SU(N)$, studies of their phase diagrams with quenched disorder, and studies of their spectral properties and doping with a small concentration of holes all provide exciting directions for future research.

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